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Superparamagnetic magnetization equation in two dimensions

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An equation for the dependence of magnetization on magnetic field in the case of two-dimensional (base plane) anisotropy has been derived. The resulting equation is expressed as an infinite series of modified Bessel functions, unlike the elementary function expressions that are applicable to the one-dimensional (axially anisotropic) and three-dimensional (isotropic) cases. Nevertheless, in the low-field limit, the series can be effectively truncated to give an approximate solution, while, in the high-field limit, an alternative expression has been derived which represents the limiting function as the field strength tends to infinity. The resulting expressions can be used to describe the superparamagnetic magnetization and susceptibility as a function of magnetic field in situations where the magnetic moments are constrained to lie in a plane, with no preferred direction within the plane. This can therefore be applied to two-dimensional structures, such as magnetic thin films, where magnetostatic energy confines the moments to the plane of the film, or to three-dimensional structures with planar magnetocrystalline anisotropy. © *2000 American Institute of Physics.* [S0003-6951(00)01433-9]

The equations describing magnetization of an uncoupled paramagnetic array of magnetic moments or an exchange coupled superparamagnetic array of magnetic moments using statistical thermodynamics have been well known for some time. In the isotropic three dimensional case,[1] which is equivalent to assuming all directions are equally probable, the equation is the Weiss modification to the classical Langevin expression

$$M = M_s[\coth(x) - 1/x], \tag{1}$$

where $x = (\mu_0 m\tilde{H})/(k_B T)$, μ_0 is the permeability of free space, M is the average projection of magnetization in the direction of external field H, $\tilde{H} = H + \alpha M$ is the effective field, M_s is saturation magnetization, m is magnetic moment, k_B is Boltzmann's constant, T is temperature, and α is the self coupling coefficient. In the one dimensional case,[2] which is equivalent to axial anisotropy, the equation is

$$M = M_s \tanh(x). \tag{2}$$

As discussed recently by Kodama[3] the forms of these equations can be used to describe superparamagnetism of nanoparticles, where m is the magnetic moment of the particle; or the classical treatment of paramagnetism ($\alpha = 0$) or ferromagnetism ($\alpha > 0$), where m is the magnetic moment of the individual atoms. The latter equation also applies to quantized magnetic moments with spin 1/2 constrained to lie in one of two possible states, ''spin up'' and ''spin down.''

However, in cases where the magnetic moments are constrained to lie in a plane, no closed form equation similar to (1) and (2) exists. This problem has become of significant technological interest with the development of magnetic structures such as thin films and multilayers for magnetoresistive devices.

This situation arises in thin film magnetic structures where magnetostatic energy confines the moments to the plane of the film. It also arises in three-dimensional structures with strong planar magnetocrystalline anisotropy, so that the moments are precluded from lying along the unique axis by magnetocrystalline anisotropy but the magnetic moments can rotate within a plane in which all directions are equivalent. Such a situation arises approximately in some materials with hexagonal crystal structures for example.

In this letter we show the derivation of an equation for the two-dimensional case and show how this can be used in the low-field limit. This equation cannot be expresssed in terms of the elementary functions, but can be expressed through modified Bessel functions or by using an infinite series. More precisely, the solution is the quotient of two infinite series, in which the numerator is the derivative of the denominator. Both these series diverge as x, and hence the ratio H/T, becomes large. However, the high-field limit of their ratio can be determined and an asymptotic expression will be derived for it in this letter by making use of l'Hopital's rule.

The first step in deriving the superparamagnetic equation for the two-dimensional case is from statistical thermodynamics. The energy of a magnetic moment m in a field H is given by $E(\theta) = -\mu_0 m\tilde{H}\cos\theta$. The probability of occupancy is $P \sim \exp[-E(\theta)/(k_B T)]$. Considering all possible orientations of magnetic moments in the plane, the following integral is obtained for the statistical sum Z:

$$Z = \int_0^{2\pi} \exp(x\cos\theta)\, d\theta = 2\pi I_0(x), \tag{3}$$

which normalizes the thermodynamical probability of the corresponding system. To evaluate the integral in (3) Sonine's[4] expansion for the modified Bessel function was used where

$$\exp(x\cos\theta)=I_0(x)+2\sum_{p=1}^{\infty} I_p(x)\cos(p\theta). \tag{4}$$

The average projection of the magnetization is then

$$M=\frac{k_BT}{\mu_0}\frac{d}{d\tilde{H}}\log Z=M_s\frac{I_0'(x)}{I_0(x)}, \tag{5}$$

where

$$I_0(x)=\sum_{s=0}^{\infty}\frac{1}{(s!)^2}\left(\frac{x}{2}\right)^{2s} \tag{6}$$

and

$$I_0'(x)=\sum_{s=1}^{\infty}\frac{s}{(s!)^2}\left(\frac{x}{2}\right)^{2s-1}. \tag{7}$$

The numerical solution of the equation requires that only a finite number of terms of the series in the numerator and denominator be used. As an example the equation with five terms is

$$\frac{I_0'(x)}{I_0(x)}\approx\frac{\dfrac{x}{(1!)^2 2}+\dfrac{2x^3}{(2!)^2 2^3}+\dfrac{3x^5}{(3!)^2 2^5}+\dfrac{4x^7}{(4!)^2 2^7}+\dfrac{5x^9}{(5!)^2 2^9}+\dots}{1+\dfrac{x^2}{(1!)^2 2^2}+\dfrac{x^4}{(2!)^2 2^4}+\dfrac{x^6}{(3!)^2 2^6}+\dfrac{x^8}{(4!)^2 2^8}+\dfrac{x^{10}}{(5!)^2 2^{10}}+\dots}. \tag{8}$$

Solutions of Eq. (8) with different numbers of terms in the series are shown in Fig. 1. From this it is clear that irrespective of how many terms are included in the series there will always be a high x (and, hence, high field) region for which the finite series approximation is not a valid physical solution.

The solutions of the equations for the one-, two-, and three-dimensional cases are shown for comparison in Fig. 2. The one-dimensional case has the highest initial differential susceptibility $\chi'=dM/dH$ and therefore approaches saturation fastest as the field H is increased. The three-dimensional case has the lowest initial differential susceptibility, since in this case the magnetic moments have the greatest freedom of choice of direction. The two-dimensional case is intermediate. The values of the initial differential susceptibility are $\chi'=\mu_0 m M_s/(nk_BT-\alpha\mu_0 m M_s)$, where n is the dimension (1,2,3).

Since divergence of the series solution is a problem as H becomes large, different approximations can be used for the low- and high-field regions. The solution must approach $M/M_s=+1$ as H approaches infinity and -1 as H approaches minus infinity. For large values of x the finite series solution M/M_s converges to 0 instead of 1, with the exact rate depending on the number of terms used. Using 18 terms, the curve can be separated into three regions: one from $x=-\infty$ to -19, the second from about $x=-19$ to 19 [over which the series solution given in Eqs. (5), (6), and (7) is valid], and the third from $x=19$ to $+\infty$. The valid range for the series solution is expanded and shifted further from the origin as more terms are added to the series approximation. A solution for high values of $|x|$ can be obtained by defining a new variable y, which is equal to $1/x$, in the series in Eq. (8). Taking the limit as x approaches plus or minus infinity is equivalent to letting y tend to zero and using l'Hopitals rule for the limit of a quotient. The following approximations

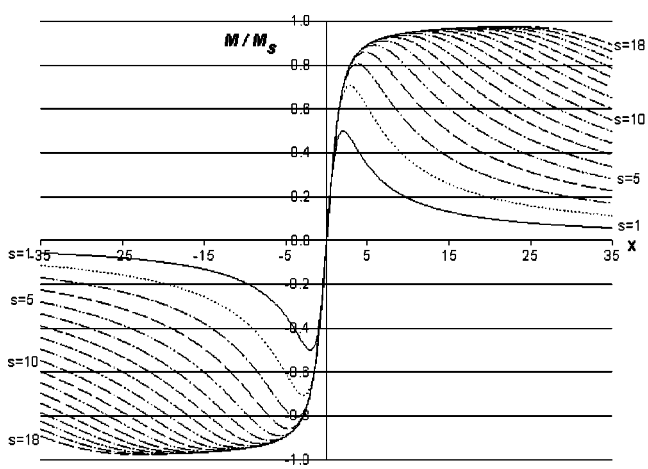

FIG. 1. Solutions of the two-dimensional Eq. (8). This shows magnetization M/M_s vs the variable x with different numbers ''s'' of terms in the series. With more terms in the series, the numerical approximation is valid over a larger range of x.

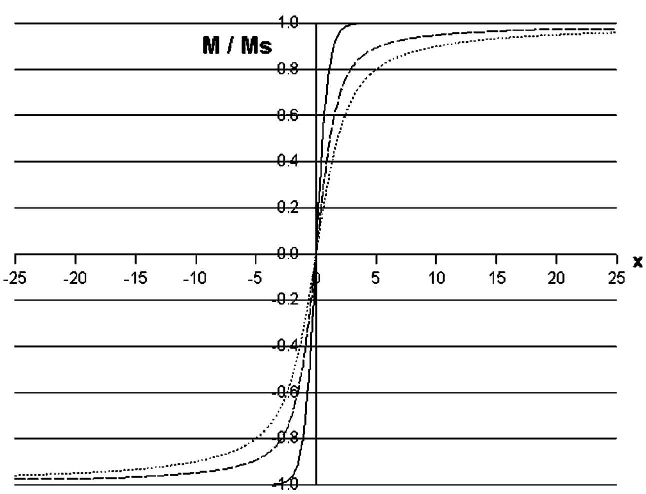

FIG. 2. Calculated initial magnetization curves M/M_s vs x for the one (solid), two (dashed) and three (dotted) dimensional cases. The one- and three-dimensional solutions are exact. The two-dimensional solution in the low-field range was obtained with 18 terms in each of the series in Eq. (8). This solution is adequate for <19. For $|x|>19$, Eq. (9) was used.

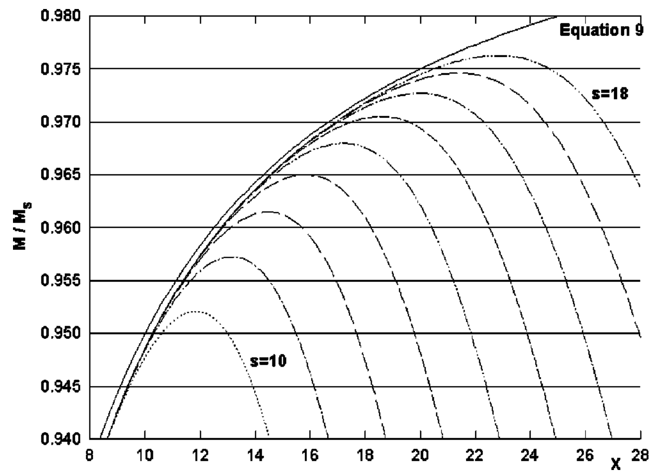

FIG. 3. Expanded view of the region of Fig. 1 in which the low-field solution [Eqs. (5), (6), and (7) with more terms of the series from $s=10$ to $s=18$] and the high-field solution [Eq. (9) with two terms] are shown. The fractional error between the two curves (M/M_s vs x) is less than 0.22% at $x=9$ with ten terms, while the fractional error is less than 0.05% at $x=19$ with 18 terms.

were found to be accurate to within a fractional error of 0.05% for values of $|x|>19$.

For $x>19$

$$M=M_s\left[1-\frac{I_0'(y)}{I_0(y)}\right]=M_s\left[1-\frac{1/(2x)+1/(16x^3)}{1+1/(4x^2)+1/(64x^4)}\right]. \quad (9a)$$

For $x<-19$

$$M=M_s\left[-1-\frac{I_0'(y)}{I_0(y)}\right]$$
$$=M_s\left[-1-\frac{1/(2x)+1/(16x^3)}{1+1/(4x^2)+1/(64x^4)}\right]. \quad (9b)$$

This approximation can be used with only two terms ($s=2$). More terms do not greatly improve the numerical precision of the solution. A simpler expression for magnetization at large values of x can be obtained using the zeroth order asymptotic expansion for $I_0(x)\sim \exp(x)/\sqrt{x}$ which leads to

$$M=M_s\left(\frac{x}{|x|}-\frac{1}{2x}\right). \quad (10)$$

A comparison of the high- and low-field solutions is shown in Fig. 3. Using 18 terms in Eq. (8) the curves are nearly coincident at $x=19$. Even though the two lines do not intersect, the fractional error between the 2 is less than 0.05%. If more terms are included in the series in Eq. (8) the difference becomes even less.

This letter has shown the development of a model equation for magnetization of a two-dimensional array of magnetic moments. It has also shown how the magnetization depends on magnetic field, temperature, magnetic moment, saturation magnetization, and self-coupling. It has been found that a single equation for this two-dimensional anhysteretic or superparamagnetic magnetization curve can be obtained. The exact solution consists of a quotient of two infinite series. The magnetization curve for this two-dimensional case lies between the one-dimensional and three-dimensional cases, both of which have exact closed form solutions.

At low values of the variable x the series solution can be calculated with a finite number of terms. For example we have shown the solution with 18 terms in each series. As the value of the variable x increases, the number of terms needed for convergence increases. Consequently for a given number of terms in the series it was found that the approximate (finite series) solution started to diverge from the correct solution. Therefore, at high values of x we have obtained an approximate solution, in which we have invoked l'Hopital's theorem for the limit of a quotient of two variables. A suitable combination of the low x and high x solutions can be used to obtain a magnetization curve over the entire range of values of x to within a chosen level of accuracy.

The solution on the M,x plane is always single valued as shown in Fig. 2. In coupled systems, for which α is nonzero, the variation of magnetization M with magnetic field H can have a different form. This arises because H is then no longer a linear function of x. This can result in elementary hysteresis loops on the M,H plane. Such behavior has been seen before.[5] The transition from linear to hysteretic M,H behavior occurs at values of $\alpha=k_BT/\mu_0 mM_s$, $2k_BT/\mu_0 mM_s$, and $3k_BT/\mu_0 mM_s$, respectively, in the one-, two-, and three-dimensional cases.

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